STATE-OF-THE-ART MULTISCALE APPROACHES FOR FLOW AND TRANSPORT MODELING:

A LITERATURE REVIEW

EXECUTIVE SUMMARY

Hydrogeologic properties vary naturally in space as a result of complex depositional, diagenetic, and structural deformational processes that evolve the aquifers. As a result, fluid flow and mass transport in aquifers are governed by parameter variations occurring at multiple scales. Accurate modeling of flow and transport calls for high-fidelity numerical models that can effectively represent and resolve all pertinent scales in both parameters and solution. Although modern site characterization techniques have made it possible to create high-resolution geologic models consisting of millions of grid cells, limitations in computing power and time often impose upper limits on the sizes of numerical flow and transport models. Upscaling, which is a conventional numerical technique used to derive equivalent block properties for coarse-resolution flow models, improves computational efficiency but smears or even hides the effects of subgrid variations. Representation of transport using a coarse-resolution flow field may underestimate the tails of solute breakthrough curves, especially in the case of strongly heterogeneous aquifers.

The current U.S. Department of Energy (DOE) Yucca Mountain site-scale saturated zone flow and transport models are represented and solved on coarse-resolution grids. The conventional wisdom is that the equivalent block-scale permeability tensor for flow and the dispersion tensor for transport can adequately compensate for the missing subgrid information.

The DOE Yucca Mountain hydrogeologic framework model and Nye County Early Warning Drilling Program provide information at much finer scales. In lieu of using global fine-resolution models to capture the effects of fine-scale variations in a brute-force manner, more elegant alternatives exist to carry forward the fine-scale information to the solutions of coarse-resolution models. This report provides an exploratory literature review of state-of-the-art multiscale modeling methods. The existing methods can be classified into heterogeneous multiscale methods and homogeneous multiscale methods, depending on whether a microscopic model is used for modeling physics at the macroscopic level. The review shows that the homogeneous multiscale methods and, in particular, the various mixed multiscale methods, are most viable for linking fine-scale information to coarse-scale models at the present time. Among the homogeneous multiscale methods, the ghost-node method of MODFLOW is a multigrid finite difference scheme for coupling coarse-resolution with fine-resolution subdomains in a numerical model; the multiscale finite element or finite volume method, however, can be easily parallelized and is capable of representing complex geologic structures.

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ACKNOWLEDGMENTS

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: All CNWRA-generated data contained in this report meet quality assurance requirements described in the Geosciences and Engineering Division Quality Assurance Manual. Sources of other data should be consulted for determining the level of quality of those data.

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1 INTRODUCTION

In recent years, there has been an enormous growth of interest in solving multiphysics problems involving multiscale numerical methods. Many problems are multiscale by nature, and there is a long history in mathematics for the study of multiscale problems using, for example, Fourier analysis and wavelet transforms (E and Engquist, 2003a). What is behind the current surge of interest is the growing need in various engineering fields to bridge solutions to problems at different scales and the ripeness of terascale computing capabilities. Scientists have been studying the macroscale problems using classic mechanics, homogenization theory, equilibrium statistical mechanics, and turbulence models for centuries. More recently, modeling the microscale problems using fundamental physical laws has gained significant popularity, driven by emerging fields such as nanoscience and molecular dynamics simulation (E and Engquist, 2003b). In this review, the macroscale generally refers to all scales where the continuum laws hold, whereas the microscale refers to substantially finer scales (e.g., nanometer scale) where the continuum theory is no longer valid.

The macroscale and microscale physics are prescribed by different governing equations. The traditional approach for solving macroscale problems has been to obtain either an analytical or numerical solution for the spatial or temporal scale of interest, while relying on the empirical constitutional relations to define macroscopic contributions of the missing scales. Examples of such constitutional relations are numerous and include Darcy's law for fluid flow in porous media, Fick's law for mass diffusion, and Fourier's law for thermal conduction. When coupled with empirical constitutional relations, the continuum equations work well for describing homogeneous systems, but become less satisfactory for complex systems, such as composite materials with complex internal boundaries, fracture dynamics, plasticity, and important regimes of turbulent flows (E and Engquist, 2003b). An important example in hydrogeology is mass transport in highly heterogeneous porous media, where semi-empirical rate-limited kinetic sorption models are sometimes used to represent the effects of neglected small-scale heterogeneities.

Hydrogeologic properties vary naturally in space as a result of complex depositional, diagenetic, and structural deformational processes that evolve the aquifers (reservoirs). The permeability of aquifers can span orders of magnitude, from impermeable flow barriers to highly permeable channels. Different hydrofacies often exhibit distinct hydraulic properties, forming complex internal boundaries and discontinuities (Koltermann and Gorelick, 1996). Advances in aquifer characterization techniques (e.g., magnetic resonance imaging, hydraulic tomography, and seismic imaging) have made it possible to obtain fine details of aquifers. Still, an accurate three-dimensional point-to-point depiction of aquifers is neither obtainable nor affordable at the scale of interest of most real projects. The limitation of computing power imposes another bottleneck. Modern geomodels range in size from 10 to 100 million cells and are growing, whereas practical industrial models can typically handle 1 million or fewer grid blocks (Gerritsen and Durlofsky, 2005; Aarnes, et al., 2006). As a result, upscaling techniques (cf., Farmer, 2002; Durlofsky, 2005; Chen and Durlofsky, 2006) are routinely used to provide homogenized or volume-averaged hydraulic parameters for numerical flow models. Modeling mass transport in upscaled or homogenized flow fields, however, is far less robust and is subject to active debate. The classic advection dispersion

equation has long been known to be insufficient for capturing scale-dependent mass transport observed at field scales. Many authors have attempted to address the effect of missing scales on mass transport via empirical closure hypotheses or stochastic simulation (e.g., Dagan, 1989; Cushman, et al., 1995; Rubin, et al., 1999; Cortis, et al., 2004; Berkowitz, et al., 2006; Fernàndez-Garcia and Gómez-Hernández, 2007). To date, however, there is no unified macroscopic framework for representing solute transport in highly heterogeneous porous media. It appears that different approaches are more or less successful in capturing field tracer experiments, as evidenced from the numerous theoretical and numerical studies done using the MADE field experiment data (Harvey and Gorelick, 2000; Baeumer, et al., 2001; Berkowitz, et al., 2006; Zhang, et al., 2007a,b). However, some of the typical concerns are (i) whether or not these theories are transferable to other sites with sparse data; (ii) how to discriminate between the approaches; and (iii) how to determine the model parameters for prediction purposes.

This literature review is motivated by uncertainties associated with the unresolved scales in the site-scale saturated zone flow and transport models for Yucca Mountain, Nevada: the site for a potential geologic repository for permanent disposal of high-level nuclear waste. The current U.S. Department of Energy (DOE) site-scale saturated zone flow and transport models are discretized into coarse numerical blocks that span hundreds of meters horizontally and tens of meters vertically (Bechtel SAIC Company, LLC, 2007). Equivalent flow and transport parameters, obtained through either model calibration or expert elicitation, are assigned to the numerical blocks. In other words, macroscopic flow and transport equations are solved for a single scale—namely, the grid scale. The missing subgrid information is often assumed to be appropriately represented by the equivalent parameters. This is not necessarily the case for highly heterogeneous porous media where the fine-scale features can cause non-Gaussian transport behavior (Painter, 1996; Wen and Gómez-Hernández, 1998; Liu, et al., 2004; Berkowitz, et al., 2006; Zhang, et al., 2007a). Well-connected, high-permeability features may indeed exist at local scales, as substantiated by recent pumping conducted at Fortymile Wash, Nevada (Reimus, 2007).

Sun, et al. (2006) recently modeled the saturated alluvial aquifer of Fortymile Wash, Nevada, through a geofacies approach, where multiple data sources (outcrop analog studies, borehole geophysics logs, and driller's cutting logs) collected from Fortymile Wash were used to directly quantify the distribution of hydrofacies in the Fortymile Wash alluvial aquifer. The main result is a two-level hierarchical hydrofacies model for the alluvial aquifer, where Level II hierarchy consists of braid-belt and paleosol facies and Level I of open-framework and non-open-framework gravels. The hierarchical model offers a parsimonious stochastic geological model for the Fortymile Wash alluvial aquifer. One of the most interesting features of the geological model is the scales it represents, ranging from meters for mean lengths of Level I facies to kilometers for Level II facies. Representing both hierarchical levels at the site-scale model is computationally challenging (Sun, et al., 2006) because of the fine resolution required. Sun and Bertetti (2007) performed stochastic simulation to assess the effects of subgrid heterogeneities using a block model. The equivalent dispersion at the block scale (equivalent to the dimensions of a typical grid block in the DOE site-scale model) was quantified through the macrodispersion tensor concept formulated in the stochastic Lagrangian transport theory (Dagan, 1989). The analyses also showed that significant spatial variability exists at the subgrid level. The fast flow channels can potentially lead to non-Gaussian mass transport behavior, raising uncertainty about radionuclide transport modeled using the classic advection–dispersion equation. To assess the effects of subgrid heterogeneities

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on site-scale flow and transport, an integrated approach is needed to take into account contributions from different scales. The main purpose of this literature study is to review state-of-the-art strategies for modeling multiscale flow and transport in porous media and assess their applicability for modeling site-scale saturated zone flow and transport at Yucca Mountain.

2 MULTISCALE MODELING

Multiscale modeling is dubbed "the best thing that has happened in applied mathematics in a long time" (E, 2007). It is expected that the 21st century will bring the integration of system software and programming tools and the seamless coupling of simulation tools for multiscale, multiphysics applications (Wheeler and Peszyńska, 2002). E and Engquist (2003a) classified the existing multiscale methods into heterogeneous multiscale methods and homogeneous multiscale methods. This classification most clearly separates different genres of multiscale methods. Two different types of problems often appear in the context of multiscale modeling
(E and Engquist, 2003b; E, et al., 2007):

- Type A. A macroscopic description is known, but ceases to be valid in localized regions in space and/or time. The microscopic models can directly model the processes happening around the singularities in the local regions.

- Type B. A macroscopic model may not be known explicitly or is too expensive to obtain, but is known to exist. There exists a set of macroscopic variables obeying a closed macroscopic model. The microscopic models can bypass *ad hoc* constitutive modeling and more accurately depict the microscopic physics.

Examples of Type A problems are crystal defects, turbulent flame fronts, and chemical systems with localized chemical reactions, where the continuum theory breaks down; examples of Type B problems include mass transport in heterogeneous porous media and in complex fluids.

Traditionally, many "multiscale" methods use the same governing equations to model physical processes at different macroscopic resolutions. These multiscale methods, such as the multigrid method and adaptive meshing, are called homogeneous multiscale methods because they all operate within the macroscopic scale. The homogenous multiscale methods are typically applied to situations where a fine-resolution grid is not feasible at the global level. Consider the mass conservation equation for steady-state fluid flow in porous media

$$\nabla \cdot (\lambda(\mathbf{x}) \cdot \nabla p(\mathbf{x})) = f(\mathbf{x}) \text{ in } \Omega \tag{1}$$

where $\lambda(\mathbf{x})$ is the mobility (i.e., permeability divided by fluid viscosity), p is pressure, f is the sink/source term, and Ω is the model domain. Here, the model parameter $\lambda(\mathbf{x})$ is obtained through averaging over the scale (volume) of interest and is generally a function of the averaging volume. The homogeneous multiscale methods are thus numerical techniques designed to fuse the fine-scale information into the solutions to coarse-resolution models. The numerical solutions improve as the model resolution

becomes finer. However, the empirical nature of the model stays, in the sense that the same governing equations are used. A presumption inherent in many homogeneous multiscale methods is that the fine-scale information is available for the numerical methods to carry forward. In practice, the estimation of fine-scale information is a complex problem by itself.

On the contrary, the heterogeneous multiscale methods recognize that problems at the macro- and microscales are governed by different physical and mathematical models. This paradigm is driven by recent developments in the so-called "first-principle" approaches, where molecular dynamics, *ab initio* quantum mechanics, or Boltzmann kinetic equations are used to resolve interactions at the microscale. The results from the microscale model are subsequently used to supplement parameters needed for the macroscale model and thus bypass the need for closure hypotheses. As a consequence, the overall solution accuracy is also improved because of the elimination of the empirical constitutional relations, whose parameters are determined by least-squares fitting of experimental data.

The vast majority of existing multiscale work in hydrogeology seems to fall into the homogeneous multiscale method category. Although pore-scale modeling has blossomed in recent years (e.g., Succi, et al., 1989; Tartakovsky and Meakin, 2006; Liu, et al., 2006; Kang, et al., 2006), studies falling into the heterogeneous multiscale method category are few (e.g., Kang, et al., 2002). Section 2.1 reviews some recent developments in heterogeneous multiscale methods. Section 2.2 reviews various homogeneous methods.

2.1 Heterogeneous Multiscale Method

There are two main parts in a heterogeneous multiscale method framework: (i) an overall macroscopic scheme for the state variable(s), where the macroscopic scheme can be either a finite volume method or a finite element method, and (ii) solution of a constrained microscopic model for estimating the missing data in the macroscopic model (E and Engquist, 2003b). The microscopic and macroscopic state variables are related to each other by the compression and reconstruction operators, which are problem dependent.

An often-used example in the literature is the gas kinetic scheme (cf., E, et al., 2007). The microscopic model in this case is the kinetic equation given by

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{1}{\varepsilon} B(f) \tag{2}$$

where the microscopic state variable f is the one-particle phase-space distribution function, $B(f)$ is a collision kernel, and ε is the mean-free path between collisions in the gas. The macroscopic state variables are the hydrodynamic variables of mass (ρ), velocity ($\mathbf{u}$), and energy densities (E), which are related to f as

$$\rho = \int f dV , \ \mathbf{u} = \frac{1}{\rho} \int f\mathbf{v}dV , \text{ and } E = \int f \frac{|\mathbf{v}|^2}{2} dV \tag{3}$$

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where *V* is the volume of integration. Equations 2 and 3 define the compression operator. If the finite volume method is chosen as the macroscopic scheme, the macroscopic fluxes at the cell boundaries become the data that need to be estimated using the microscopic model Eq. (2), subject to certain constraints.

The lattice Boltzmann method has gained popularity in studying pore-scale fluid flow in the last two decades. Linking the lattice Boltzmann method to macroscopic flow in heterogeneous porous media, however, is still under active research. It is well known that the lattice Boltzmann method can recover the correct continuity and Navier-Stokes equations. Kang, et al. (2002) proposed a unified lattice Boltzmann method for flow in multiscale porous media. In their study, the microscopic model was the discrete lattice Boltzmann equation for the particle velocity distribution function. The macroscopic porous media model was a modified Navier-Stokes equation originally proposed by Freed (1998). The density and macroscopic velocity were related to the weighted averages of microscopic particle velocities. The key was introducing an external force into the macroscopic model by altering the local and instantaneous velocity during the particle collision step. The nodal permeability tensor is required to calculate the external force. Kang, et al. (2002) demonstrated the unified lattice Boltzmann method for several synthetic problems, including a 16 × 16-m [52.5 × 52.5-ft] heterogeneous random field and a single fracture system. The lattice Boltzmann method results showed good performance and were not restricted to low Reynolds numbers, as required for the correct application of Darcy's law.

Some potential limitations of the lattice Boltzmann method and other heterogeneous multiscale methods for macroscopic porous flow and transport are

- The subject is relatively new and existing field-scale applications are few.
- The underlying permeability field is required. In practice, the uncertainty in permeability can easily offset the accuracy gained from using the "first-principle" microscopic models, defeating the original purpose of using the bottom-up multiphysics approach.
- Most demonstrations so far are limited regular grids, and the computational burden can be overwhelming without access to large-scale computing facilities.

2.2 Homogeneous Multiscale Methods

The traditional homogeneous multiscale methods are multigrid methods, domain decomposition, wavelet-based methods, and adaptive mesh refinement methods (cf., E, et al., 2007). These methods make it possible to embed fine-resolution models in coarse-resolution models. Simply speaking, multigrid methods and adaptive mesh refinement methods are a group of algorithms for solving differential equations using a hierarchy of discretizations so that submodels of different resolution can coexist in a computational domain. The domain decomposition methods split the original computation domain into smaller subdomains so that the solution for each subdomain can be obtained efficiently via parallel computing. The domain decomposition methods can be used in combination with multigrid methods in parallel computing. The wavelet methods apply a mathematical transformation to divide a given function into different frequency components and study each component with a resolution that matches its scale. This report focuses on some multiscale numerical schemes that appear in more recent hydrogeological and reservoir simulation literature. The reservoir simulation

literature contains some refined and theoretically advanced ideas for superimposed multigrid methods, linking overlapping fine- and coarse-grid solutions. Table 1 summarizes several methods.

Table 1. Summary of Some Homogeneous Multiscale Numerical Schemes	
Method	**Comments**
Multiscale Finite Element*	Construct basis functions to represent the effects of fine-scale features in coarse-resolution finite element models. More specifically, the basis functions for coarse elements incorporate subgrid features. Localization is achieved by boundary condition assumptions for the coarse elements. Does not conserve mass locally.
Mixed Multiscale Finite Element†	Similar to Hou and Wu.* However, mass-conservative velocity fields are provided on the coarse grid as well as on the underlying fine grid for nonsink/source coarse blocks.
Subgrid Upscaling‡§	Fine-scale effects are localized by a boundary condition assumption at the coarse element boundaries via numerical Green's function. A locally mass conservative technique.
Mixed Mimetic MultiscaleMethods for Corner-Point Grids§‖	Variant of Chen and Hou.† Yields globally and locally mass conservative velocity field. The corner-point grid is industry-standard for modeling complex petroleum reservoir geology.
Multiscale Finite Volume Method¶	A finite-volume method that conserves mass both globally and locally, treats permeability tensors correctly, and can be easily applied to existing finite-volume codes.
Stochastic Variation Multiscale Method#	A stochastic version of the variation multiscale method. Uses a support-space/stochastic Galerkin approach and the generalized polynomial chaos expansion approach for input–output uncertainty representation.
Multiblock Mixed Finite Element Method**††	Uses a mortar finite element boundary space to connect nonoverlapping blocks of different grid geometry together, while ensuring local mass conservation across the grid interface. Can be combined with domain decomposition.
Ghost Node Local Grid Refinement§§	An extension of the traditional telescopic finite-difference refinement. The method couples the coarse grid (parent) and fine grid (children) by sharing nodes and iteratively updating the right-hand side of the matrix equations to ensure that heads and fluxes are consistent between both grids. The boundaries of the child grid should be carefully selected to be located where the parent grid is able to adequately represent the hydraulics—generally regions of small variations in hydraulic gradient. The notion of "ghost" or "worker" nodes is widely used in mixed finite element works.

*Hou, T. and X.H. Wu. "A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media." *Journal of Computational Physics*. Vol. 134. pp. 169–189. 1997.
†Chen, Z. and T. Hou. "A Mixed Multiscale Finite Element Method for Elliptic Problems with Oscillation Coefficients." *Mathematics of Computation*. Vol. 72. pp. 541–576. 2003.
‡Arbogast, T. "Numerical Subgrid Upscaling of Two Phase Flow in Porous Media." Technical Report, Texas Institute for Computational and Applied Mathematics. Austin, Texas: The University of Texas at Austin 1999.
§Arbogast, T. and K. Boyd. "Subgrid Upscaling and Mixed Multiscale Finite Elements." *SIAM Journal on Numerical Analysis*. Vol. 44, No. 3. pp. 1,150–1,171. 2006.

Table 1. Summary of Some Homogeneous Multiscale Numerical Schemes (continued)

‖Aarnes, J.E., and Y. Efendiev. "A Multiscale Method for Modeling Transport in Porous Media on Unstructured Corner-Point Grids." Proceedings of CMWR XVI. Copenhagen, Denmark: Technical University of Denmark. 2006.

¶Jenny, P., S.H. Lee, and H.A. Tchelepi. "Multiscale Finite-Volume Method for Elliptic Problems in Subsurface Flow Simulation." *Journal of Computational Physics*. Vol. 187. pp. 47–67. 2003.

Velamur, A.B. and N. Zabaras. "Variational Multiscale Stabilized FEM Formulations for Transport Equations: Stochastic Advection-Diffusion and Incompressible Stochastic Navier-Stokes Equations." *Journal of Computational Physics*. Vol. 202. pp. 134–153. 2005.

**Arbogast, T., L.C. Cowsar, M.F. Wheeler, and I. Yotov. "Mixed Finite-Element Methods on Non-Matching Multiblock Grids." *SIAM Journal on Numerical Analysis*. Vol. 37. pp. 1,295–1,315. 2000.

††Wheeler, M.F. and M. Peszyńska. "Computational Engineering and Science Methodologies for Modeling and Simulation of Subsurface Applications." *Advances in Water Resources*. Vol. 25. pp. 1,147–1,173. 2002.

§§Mehl, S., and M.C. Hill. "MODFLOW-2005, Documentation of Shared Node Local Grid Refinement (LGR) and the Boundary Flow and Head (BFH) Package." U.S. Geological Survey Techniques and Methods Report 6-A12. 2005

All methods reviewed in Table 1, except Items 3 and 8, are mixed finite element methods that are based on a variational principle to express an equilibrium condition that can be satisfied locally on each finite element. For elliptic problems, the mixed finite element formulation involves solving a scalar variable and the flux simultaneously. In principle, approximating spaces for the mixed finite element method can be chosen to satisfy three properties: local mass conservation, continuous fluxes, and the same order of convergence for both the scalar variable and the flux (Wheeler and Peszyńska, 2002).

The calculation of basis functions constitutes the core of mixed finite element methods. For each block interface in the coarse-grid model, a corresponding basis function Ψ_{ij} is used to incorporate the local impact of subgrid permeability (K) variations, which is related to an unknown function Φ_{ij} through Darcy's law

$$\Psi_{ij} = -K\nabla\Phi_{ij} \tag{4}$$

The basis function Ψ_{ij} and the unknown function Φ_{ij} are found by solving a local elliptic problem subject to boundary conditions (cf., Aarnes, et al., 2005). Ideally, the imposed boundary conditions should approximate the true flow conditions experienced by the coarse block in the global model, which can be time and flow dependent.   Enforcing unit flux conditions across the coarse block boundary can yield much better numerical results than the linear or constant pressure conditions (Aarnes, et al., 2005; Jenny, et al., 2003). In addition, if a mass conservative method is used to compute basis functions, the mixed finite element approach gives mass conservative velocity fields for both the coarse grid and the underlying fine grid.

The computational complexity of using a mixed multiscale finite element (or finite volume) method is comparable to that of solving the full problem on a fine grid with an efficient linear solver. The most intensive part of the computation is related to basis function calculation, although the process can be parallelized easily because the basis functions are independent from each other. So why use the multiscale finite-element method for single phase problems if its computational complexity is proportional to

solving a full fine-grid problem? Aarnes and Efendiev (2006) gave several justifications.
First, the multiscale finite element method (or many other methods listed in Table 1) can
potentially solve very large-scale problems on the parallel computing platform. It is true
that parallel computing methods such as domain decomposition are often used directly
to solve the fine-grid models. However, domain decomposition may give mass balance
errors. Second, uncertainty analyses of boundary conditions and source terms require
repeated model runs for a given fine-scale structure (e.g., permeability field). The basis
functions only need to be constructed once, offering significant savings in computing
time and memory requirement of subsequent runs. The basis functions have to be
reconstructed whenever the underlying permeability field changes, as in the case of
simulating the effects of the fine-scale permeability variability. However, the geologic
model involving multiscales is assumed known at the outset when applying the
multiscale methods. The combination of mixed finite element and multiblock offers an
option to use different discretization at different subdomains of a model (Wheeler and
Peszyńska, 2002).

The ghost-node finite-difference method developed by Mehl and Hill (2002) merits more
discussion here. In this method, the boundary conditions of the parent and child grids
are linked through the "ghost" or "slave" nodes, and the models are solved iteratively
until both fine- and coarse-grid solutions converge. The convergence rate is generally
expected to be quadratic. The idea shares and builds on related methods by Szekely
(1998) and Arbogast, et al. (2000). The coding in a MODFLOW-compatible module by
Mehl and Hill (2005) makes the ghost node method practical to apply. Linking the
boundary conditions is conceptually straightforward if one is familiar with the MODFLOW
boundary condition approaches. The coarse-grid has specified flow boundary
conditions. Ghost nodes are located along a trace (two-dimensional) or plane (three-
dimensional) on the coarse-grid boundary cells and mirror the fine-grid nodes. This
placement allows heads at ghost nodes to be interpolated from heads at coarse-grid
boundary nodes. The ghost nodes are, in turn, used as fixed-head in head-dependent
boundary conditions on the fine grid. More rigorous testing under more heterogeneous
conditions with complex boundary conditions is needed, as are introduction and testing
of approaches for incorporating the simulation of transport with mechanical dispersion.

As mentioned before, a crucial assumption in the homogeneous multiscale methods
mentioned here is that the fine-scale information is available and is largely deterministic.
Field measurements are usually sparse and often come in different scales and forms.
As a result, inverse methods are used to convert multiscale data to the scale of interest
during site characterization and history matching. The problem is often ill-posed
because the downward mapping from coarse scale to fine scale is nonunique and
statistical techniques are used to impose regularity constraints during downscaling
(Yoon, et al., 2001; Efendiev, et al., 2005; Efendiev and Hou, 2007).

Much less work has been done in coarse-scale representation of transport (Gerritsen
and Durlofsky, 2005; Efendiev and Durlofsky, 2003; Rubin, et al., 1999). Instead of
inflating the dispersion tensor to compensate for subgrid variability on solute transport, a
straightforward strategy is to reconstruct the fine-scale velocity field from the solution of
the multiscale solver and solve for solute transport using particle tracking.

3 SUMMARY AND CONCLUSION

It is important to take the multiscale nature of geologic formations into account when building field-scale flow and transport models. DOE's current Yucca Mountain site-scale saturated zone flow and transport models are represented and solved on a coarse-resolution grid. Recent research suggests that fine-scale variations may lead to non-Gaussian transport behavior. In this report, existing multiscale methods are reviewed according to their relevance to field-scale flow and transport in porous media. The heterogeneous multiscale framework originally proposed by E and Engquist (2003b) is used to classify existing methods into heterogeneous multiscale methods and homogeneous multiscale methods, where strictly speaking, the latter is a subclass of the former.

The main findings are
- The heterogeneous multiscale methods represent a relatively new area of research in computational physics. The microscopic models are used to simulate physics at the microscopic level, which in turn, yields accurate data or parameters needed by the macroscopic models. The idea is novel and promising. However, most applications are restricted to proof-of-concept examples. Field demonstrations are still to be seen.

- The homogenous multiscale methods include a wide array of different theoretical and numerical approaches. These methods generally assume that the same set of governing equations is applicable to different continua within the macroscopic scale.
  — The mixed multiscale finite element (or finite volume) method is flexible enough to represent complex geometries encountered in real problems and offers more advantages than the traditional upscaling approach. The basis functions require a significant computation overhead to obtain. However, the computation can be parallelized because basis functions are independent.
  — The ghost-node method implemented in the latest MODFLOW package is essentially a multigrid method for the finite-difference scheme. The ghost-node method may be used to embed a fine-scale model into a coarse-scale numerical model.

In summary, the mixed multiscale methods and the ghost-node method are the most viable computing techniques for carrying forward the fine-scale information to the site-scale flow model. The advantage of the finite-element method is that it handles complex geometries, which can be important to represent the contacts of different geologic units. Forward modeling using multiscale methods may reduce uncertainties associated with the coarse-resolution flow and transport models.

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